Scientific Research and Essays Vol. 6(13), pp. 2710-2719, 4 July, 2011
Available online at http://www.academicjournals.org/SRE
DOI: 10.5897/SRE10.1190
ISSN 1992-2248 ©2011 Academic Journals

Full Length Research Paper

Statistical clustering of maxillary dental arches

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Accepted 30 May, 2011

The purpose of this study was to define a procedure for grouping Malaysian dental arches into clusters by applying the agglomerative hierarchical clustering (AHC) method. Standardized digital images of maxillary dental casts of 170 subjects were used to measure the distance joining left and right hamular notches, *a*, and the perpendicular distance between this line and the incisive papilla, *b*. Coefficients of the fitted quadratic curve $(\alpha_2, \alpha_1 \text{ and } \alpha_0)$ were calculated using selected landmarks on the casts. The variables $a, b, \alpha_2, \alpha_1 \text{ and } \alpha_0$ were then used to represent the shape of each dental cast. Subsequently, casts were randomly divided into 2 subsamples; control and test samples. The AHC method was applied to the control sample to establish clusters. To verify the clusters formed, 40 test samples were assigned to the clusters. The number of acceptable clusters was established when no cluster had less than 4 members (10% of the test samples). The total number of members in all formed clusters was at least 36 (90% of the test samples) and the margin of error, *h* was 5 mm (least acceptable value). Using the AHC method, maxillary dental arches may be grouped into 3 clusters as defined by the median values of the proposed shape parameters investigated; (46.88 mm, 47.83 mm, 5.12, 0.55,-57.20), (47.31 mm, 43.21 mm, 4.89, 0.11, -53.52) and (51.51 mm, 50.09 mm, 4.85, 0.05, -60.74) respectively.

Key words: Clustering method, maxillary dental arch, maxillary dental arch size and shape.

INTRODUCTION

Dental arches have been characterized by simple qualitative descriptions or mathematical methods, depending on the objective of the study and different anatomical landmarks and measurement techniques used (Al Harbi et al., 2008; Burris and Harris, 2000; Cruz et al., 1995; Ferrario et al., 1994; Hao et al., 2000; Pepe, 1975; Raberin et al., 1993; Richards et al., 1990). Interest in clustering the arch form arose from clinical experience in finding suitable impression trays for impression making (Bomberg et al., 1985; Carrotte et al., 1998). A sufficient amount of space must be present between the impression tray and oral tissues to allow a certain thickness of impression material so that any dimensional changes attributed to the impression material may be minimized. A dental impression is most accurate when there is a minimal and even thickness (2 to 4 mm) of impression material between impression tray, the teeth and oral tissues to be registered in the impression (Millstein et al., 1998). As a result of this, more material may be required when using stock trays which are not well-fitting than when using well-fitted custom trays (Christensen, 1994).

From a review of the literature there appears to be no scientific basis for the design of stock impression trays. Multiple sizes are made by different manufacturers to accommodate a range of mouth sizes, although trays are generally U-shaped. Accurate casts can be made with either stock trays or specially made individual custom trays, as long as the trays fit the dental arches well (Mendez, 1985; Thongthammachat et al., 2002). In this study, the immediate concern was whether the Malaysian

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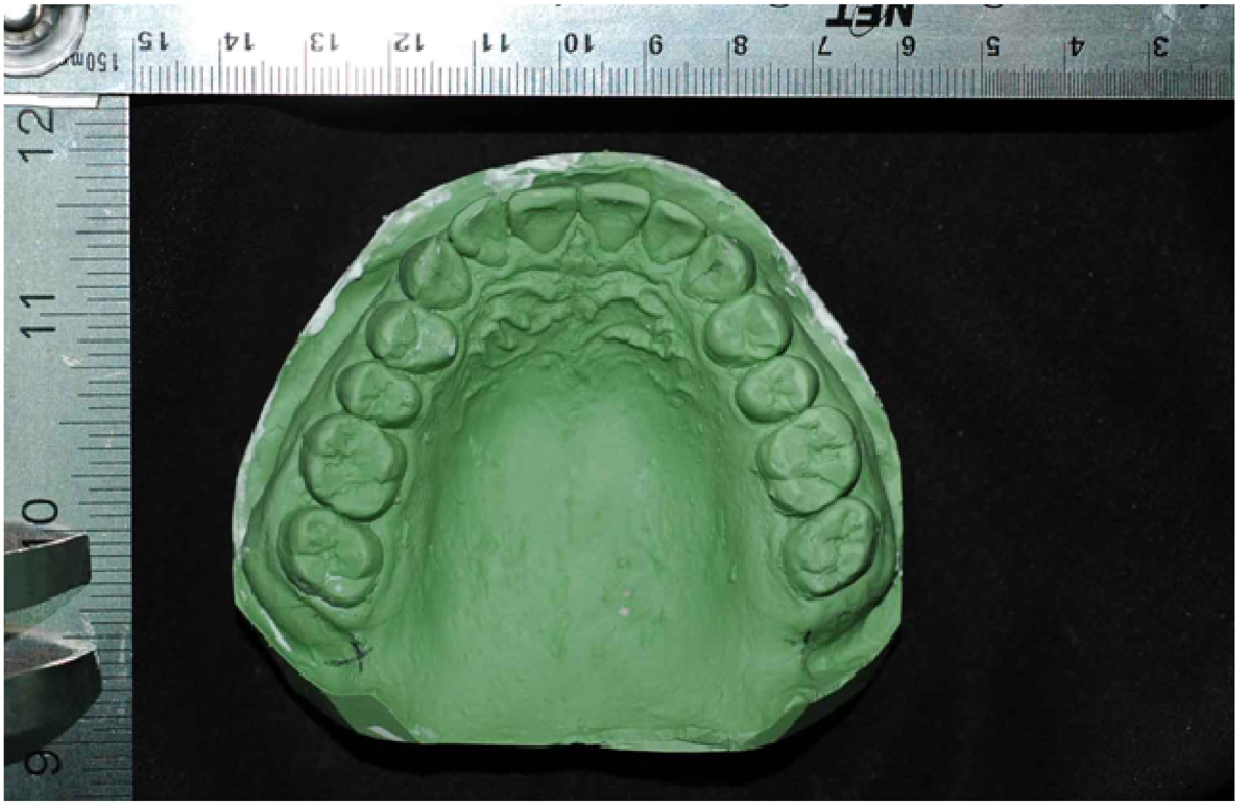


Figure 1. Standardized position of the cast when its digital image was captured. Two metal rulers were positioned on a plane parallel to the occlusal plane for calibration of the measurements.

population is homogeneous with respect to arch form, and whether the stock trays available commercially are adequate to be used for the Malaysian population. In a multiethnic society, it is reasonable to assume that possible variations in arch size and shape exist in the population (Burris and Harris, 2000; Diwan and Elahi, 1990; Mack, 1981; Younes, 1984). Investigating individuals with similar arch form would establish clusters from which information can be derived to develop impression trays appropriate for a specific population. Therefore, the purpose of this study was to use information obtained from dental casts to find possible groups of arch forms according to shape.

MATERIALS AND METHODS

The study sample was 170 maxillary dental casts of subjects aged between 18 and 36 years. The subjects comprised of 3 main Malaysian ethnic groups, namely the Malays (49 women and 39 men), Chinese (24 women and 21 men) and Indians (20 women and 17 men). All subjects had well aligned maxillary anterior teeth with minimum attrition. Subjects were excluded if they had a history of orthodontic treatment, anterior restoration or a fixed dental prosthesis in the maxilla or mandible.

Impressions of the maxillary arches of the subjects were made with irreversible hydrocolloid (Duplast fast set alginate impression material; Dentsply Dental Co Ltd, Tianjin, China). Impressions were cast using type III dental stone (Moldano; Heraeus Kulzer GmbH, Hanau, Germany). Standardized digital images from the occlusal surfaces of the casts were captured by digital camera (Nikon D70s; Nikon Corp, Tokyo, Japan). The camera-object distance was fixed at 50 cm to ensure distortion free images. Two metal rulers fixed perpendicular to each other and positioned on a plane parallel to the occlusal plane were used as frames for standardization and calibration of the measurements (Figure 1).

The images were analyzed using MATLAB software (version R2009b, The MathWorks Inc., USA). A standard image processing technique was applied where a calibration method converts all measurements in terms of number of pixels into millimeters. Three anatomical landmarks (incisive papilla, right and left hamular notches) were used as reference points for each cast (Petričević et al, 2005; Petričević et al. 2006). The line joining the two hamular notches was used geometrically as the Cartesian x-axis, while the line perpendicular to the x-axis passing through the incisive papilla was defined as the y-axis. The point where both axes meet was defined as the origin of the coordinates. A quadratic curve was fitted to the coordinates of 14 points on each arch. The points selected were: the midpoint of the incisal edge of the central and lateral incisors, the canine tips, the midpoint of the buccal cusp tips of the first and second premolars, and the mesiobuccal cusp tips of the first and second molars (Burris and Harris, 2000) (third molars were excluded) (Figure 2). The distance between the two hamular notches, *a*, distance between the incisive papilla to the origin, *b* and the fitted quadratic coefficients α_2, α_1 and α_0 were collectively used to represent the shape of each dental cast. Henceforth, the i^{th} dental cast was represented by the vector

$(a_i, b_i, \alpha_{2i}, \alpha_{1i}$ and $\alpha_{0i})$ where i= 1,…,170.

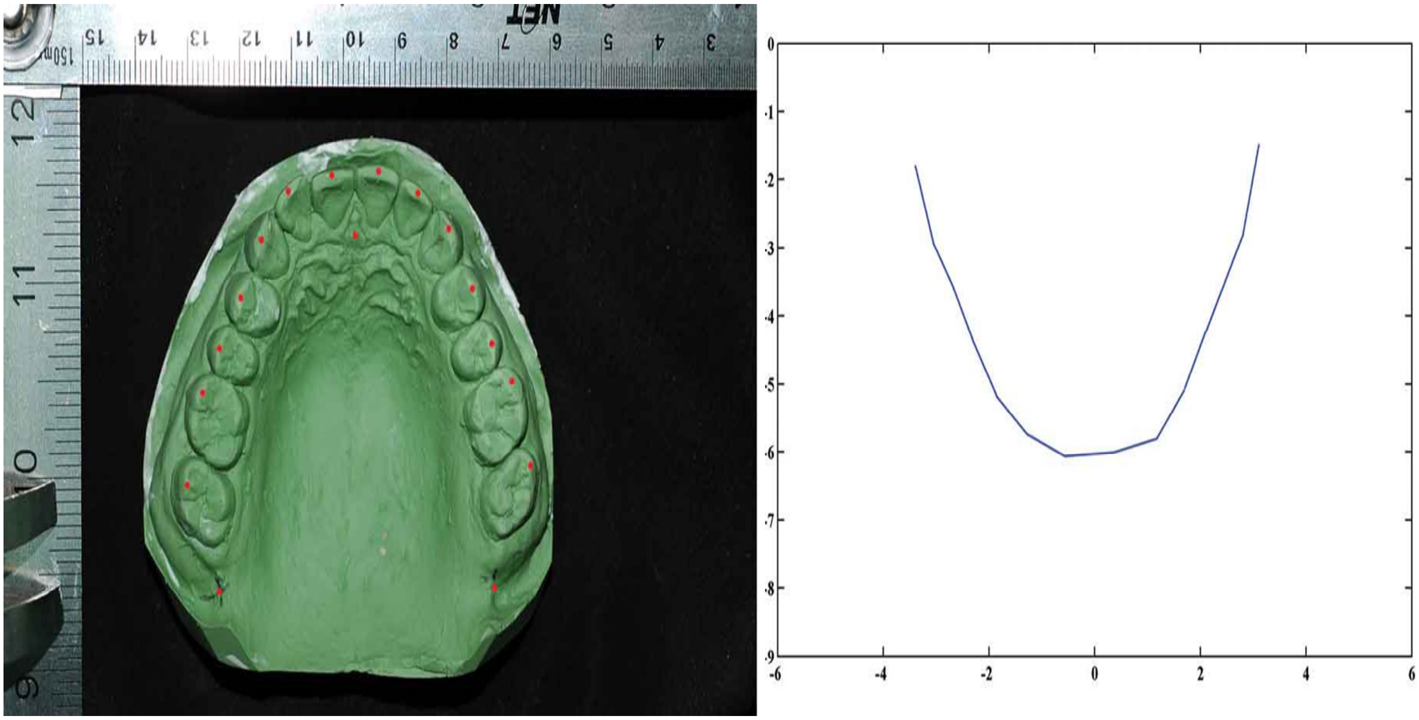


Figure 2. Representation of the selected points from the cast to the cartesian system.

Boxplots were used to determine outliers for each of a, b, α_2, α_1 and α_0 , respectively (Anderberg, 1973). Casts with outliers detected were eliminated from the whole sample. Subsequently, the casts were rearranged following a computer generated list of random numbers. Then, they were randomly divided into the control sample (to estimate number of clusters) and test sample (to estimate appropriateness of the formed clusters).

Using the control samples, a measure of distance or separation between the k^{th} dental cast and the j^{th} dental cast is as follows (Anderberg, 1973):

$$d(k,j)=\sqrt{(a_k-a_j)^2+(b_k-b_j)^2+(\alpha_{2k}-\alpha_{2j})^2+(\alpha_{1k}-\alpha_{1j})^2+(\alpha_{0k}-\alpha_{0j})^2}$$

The whole set of distances may be expressed in the matrix:

$$D(0,k,j)=\begin{bmatrix} 0 & & & & \\ d(2,1) & 0 & & & \\ d(3,1) & d(3,2) & 0 & & \\ \vdots & \vdots & & \ddots & \\ d(n,1) & d(n,2) & \ldots & d(n,n-1) & 0 \end{bmatrix}.$$

The first step in the AHC method was to merge two dental casts with the smallest $d(k,j)$ value between them into the same group. The distance between this new group and the remaining original dental casts was then redefined using one of the following methods:

M1. Single linkage method; $d(k,j)$ = minimum distance between dental casts in cluster-*k* and cluster-*j*.
M2. Average linkage method; $d(k,j)$ = average distance between all pairs of dental casts in cluster-*k* and cluster-*j*.
M3. Centroid linkage method; $d(k,j)$ = distance between centroid of cluster-*k* and cluster-j.
M4. McQuitty's linkage method; $d(k,j)$ = the average distance of d(*k,l*) and d(*j,l*), given three cluster-*k,* cluster-*j* and cluster-*l"*.
M5, Median linkage method; $d(k,j)$ = median distance between all pairs of dental casts in cluster-*k* and cluster-*j*.
M6. Ward's linkage method; $d(k,j)$ = minimum error sum of squares of cluster-*k* and cluster-*j*.
M7. Complete linkage method; $d(k,j)$ = maximum distance between dental casts in cluster-*k* and cluster-*j*.

A description of these methods can be found in Anderberg (1973), Everitt et al. (2011), and Minitab (1999).

Using one of the above methods, the set of distances after the merger would be found in the matrix $D(1,k,j)$. The next step in the AHC method was to combine two dental casts or two groups of dental casts with the smallest $d(k,j)$ obtained from the matrix $D(1,k,j)$. This process of combining two groups and merging their characteristics was repeated until all dental casts were placed in one large group. The result of this hierarchical cluster analysis is shown graphically in a dendrogram (Figure 3), where all the samples are listed and the level of similarity showing how any two clusters were joined are indicated (Mardia et al. 1979). In Figure 3, the horizontal axis indicates the position of the dental casts (relative to each other) whilst the height of the vertical axis is a measure of the disparity among the casts. The similarity level at the i^{th} merger of clusters is defined as (Minitab, 1999).

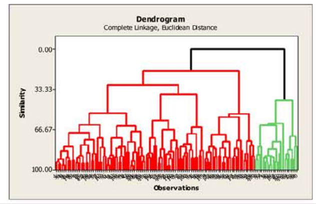
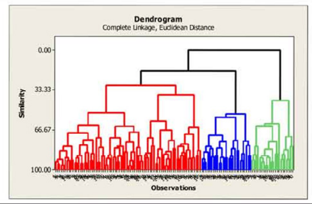
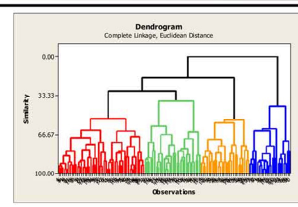
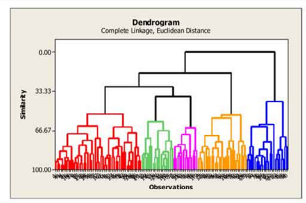
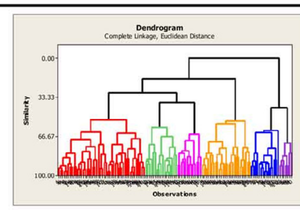
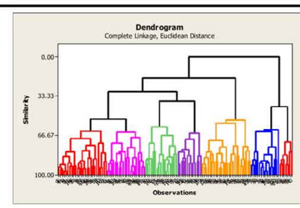
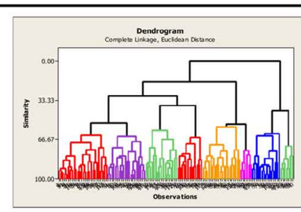
Number of clusters	Similarity level (%)	Dendrogram
2	1 to 17	
3	18 to 29	
4	30 to 37	
5	38 to 42	
6	43 to 53	
7	53.5	
8	54 to 56	

Figure 3. Dendrograms showing number of clusters at different cut-off levels obtained from complete linkage method**.**

$$S(i) = \left(1 - \frac{\min\{\, d(k, j) \text{ in } D(i, k, j)\}}{\max\{\, d(k, j) \text{ in } D(0, k, j)\}}\right) \text{x } 100\%$$. A large $S(i)$ value suggests dental cast-*k* and dental cast-*j* (or two groups of dental casts) have similar arch shape. The number of clusters is chosen by selecting the height of the vertical axis which

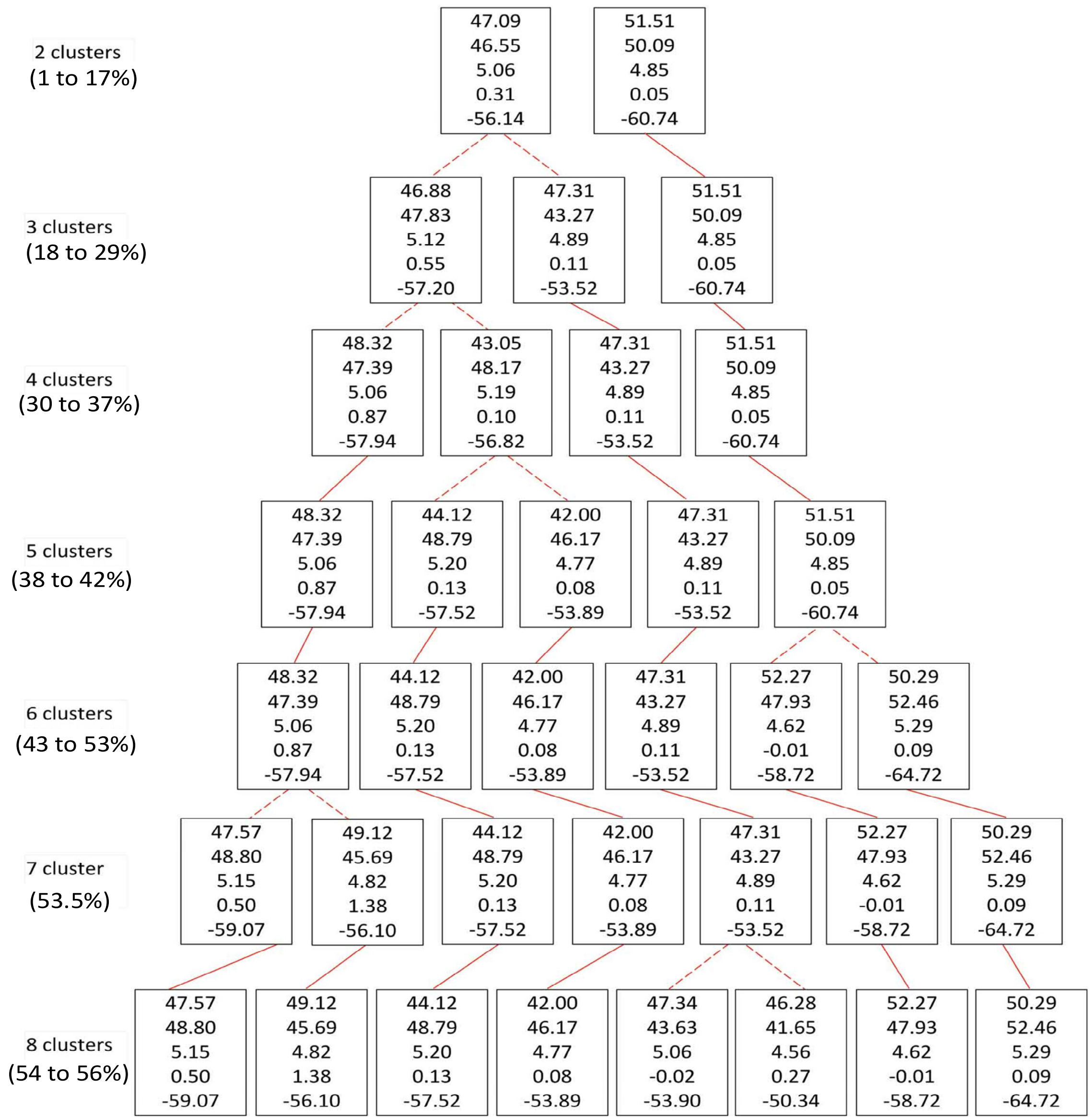


Figure 4. The pyramid of cluster boxes where each cluster is represented by the vector of medians $\begin{bmatrix} a^* \\ b^* \\ \alpha_2^* \\ \alpha_1^* \\ \alpha_0^* \end{bmatrix}$ for selected similarity levels using the complete linkage method.(Broken red line represents possible split of cluster / fusion of cluster; continuous red line suggests no change in cluster).

represents the cut-off point.

The medians of a, b, α_2, α_1 and α_0 were denoted as $a_j^*, b_j^*, \alpha_{2j}^*, \alpha_{1j}^*, \alpha_{0j}^*$ respectively and were collectively used to represent a group. Each group may also be graphically represented by a box containing the medians for a given similarity value. The information concerning similarity level with respect to number of clusters formed is displayed as a pyramid of boxes of medians (Figure 4). The definitive number of clusters formed from the control sample, will depend on a further process of assigning members of the test sample into the formed clusters. This was carried out as follows:

The criteria for the k^{th} test sample $(\hat{a}_k, \hat{b}_k, \hat{\alpha}_{2k}, \hat{\alpha}_{1k}, \hat{\alpha}_{0k})$ to be accepted into the j^{th} cluster $(a_j^*, b_j^*, \alpha_{2j}^*, \alpha_{1j}^*, \alpha_{0j}^*)$ were:

a. $\left| b_j^* - \hat{b}_k \right| \le h$, the absolute difference between the median *b*-value and test *b*-value,

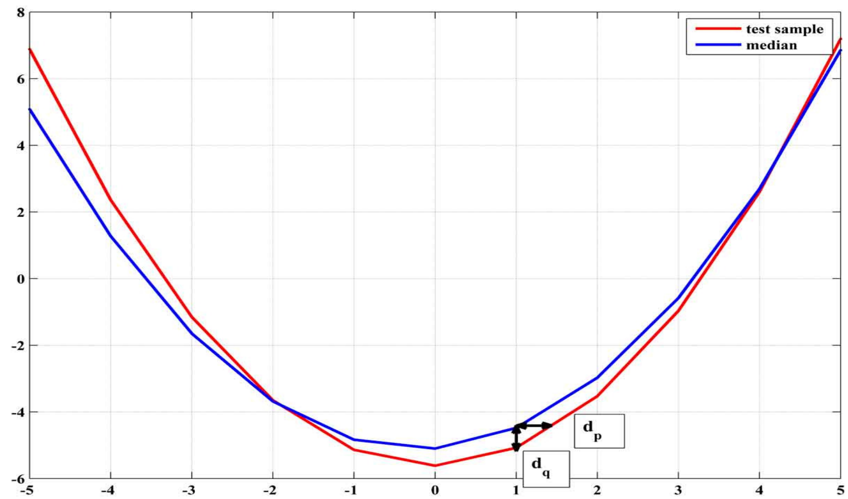


Figure 5. Superimposition of the median and test sample curves to obtain differences between the two quadratic curves.

b. $\left|a^*_j - \hat{a}_k\right| \leq h$, the absolute difference between the median *a*-value and test *a*-value, and

c. $\sum d_q + \sum d_p \leq (m+i)h$, the sum of the absolute differences between two quadratic curves $y^*_j = \alpha^*_{2j}x^2 + \alpha^*_{1j}x + \alpha^*_{0j}$ (median curve) and $\hat{y}_k = \hat{\alpha}_{2k}x^2 + \hat{\alpha}_{1k}x + \hat{\alpha}_{0k}$ (Figure 5).

d. The maximum error was chosen to be $(m+i)h$ because it is necessary to ensure that when making dental impressions, a minimal and even thickness of impression, material should exist throughout the maxillary arch, where *h* is the vertical difference between the two curves at a given point on the horizontal axis. The number of vertical differences is *m* and the number of horizontal differences is *i*, such that:

$$\sum_{q=1}^{m} d_q = \left|y_{j1} - \hat{y}_{k1}\right| + \left|y_{j2} - \hat{y}_{k2}\right| + \ldots + \left|y_{jm} - \hat{y}_{km}\right|$$ and

$$\sum_{p=1}^{i} d_p = \left|x_{j1} - \hat{x}_{k1}\right| + \left|x_{j2} - \hat{x}_{k2}\right| + \ldots + \left|x_{ji} - \hat{x}_{ki}\right|.$$

When the conditions above were satisfied, the k^{th} test sample $(\hat{a}_k, \hat{b}_k, \hat{\alpha}_{2k}, \hat{\alpha}_{1k}, \hat{\alpha}_{0k})$ was said to belong to cluster *j*.

Calculations of $\sum_{q=1}^{m} d_q$ and $\sum_{p=1}^{i} d_p$ were done for selected points given in the range of [-20, 20] and [-45, -30] for *x* and *y* respectively, as they were considered as being representative of the actual length and width of the casts.

RESULTS

Box plots of values of a, b, α_2, α_1 and α_0 of 170 casts showed existence of outliers in 6 casts. The outliers were removed to ensure the clustering methods yield consistent groupings. Subsequently, the study sample was randomly divided into the control samples (124 casts) and test samples (40 casts).

The descriptive statistics (mean, standard deviation, minimum, maximum and median values) of the linear (a and b) and non-linear (quadratic coefficients) measurements are listed in Tables 1(a) and 1(b) for the control sample and Tables 2(a) and 2(b) for the test sample, respectively.

A summary of clusters formed from the control sample using methods M1 to M7 with selected similarity values are shown in Table 3. The problem of misfit of impression trays with patients' mouths suggests that there should be at least 2 clusters of dental arches. It is seen that only with the complete linkage method was there a realistic number of groups or clusters of shapes of dental arches (2 to 6) for a similarity level of up to 50%.

Figure 3 shows the possible number of clusters of the control sample that may be obtained using the complete linkage method. Figure 4 shows the median value of (a, b, α_2, α_1 and α_0) corresponding to the clusters showed in Figure 3. Using the test samples, Table 4 shows cluster membership as defined by *h* and similarity level. As the optimal thickness of an impression material in dental restorative procedures should be between 2 and 4 mm on either side of a tooth, the use of *h* to be 5 mm in this study was most appropriate. In this study, any cluster with less than four members (10% of samples) was discarded in order to avoid small cluster membership. To avoid having many outliers, 90% of all samples must be captured by all clusters. Consequently, the test samples strongly suggest the existence of 3 groups when *h* = 5 mm at similarity values between 18 and 29% (Table 4). Note that this study may be repeated with larger sample size and applying more stringent condition, for example, 95% of all samples must be captured by all clusters formed.

Table 1a. Mean, median and standard deviation values and range of linear measurements for the control samples.

Variable	Mean (mm) (SD)	Minimum (mm)	Maximum (mm)	Median (mm)
a	47.59 (3.51)	38.73	56.42	47.66
b	47.18 (3.00)	39.69	54.28	47.43

Table 1b. Mean, median and standard deviation values and range of quadratic coefficients of the non-linear measurements for the control samples.

Variable	Mean (SD)	Minimum	Maximum	Median
α_2	5.00 (0.58)	3.96	6.57	4.94
α_1	0.37 (1.49)	-3.36	4.29	0.21
α_0	-57.07 (3.46)	-66.06	-49.75	-57.03

Table 2a. Mean, median and standard deviation values and range of linear measurements for the test samples.

Variable	Mean (mm) (SD)	Minimum (mm)	Maximum (mm)	Median (mm)
a	48.74 (3.58)	41.55	56.32	48.25
b	46.89 (3.45)	39.77	52.76	46.89

Table 2b. Mean median and standard deviation values and range of quadratic coefficients of the non-linear measurements for the test samples.

Variable	Mean (SD)	Minimum	Maximum	Median
α_2	4.94 (0.64)	3.41	6.37	5.02
α_1	0.58 (1.64)	-2.22	4.89	0.36
α_0	-57.05 (4.54)	-65.70	-48.38	-57.73

DISCUSSION

Dental practitioners are often confronted with the problem of finding an impression tray that fits a dentate patient. The most recurrent problem seen is the eccentric orientation of the tray to the arch on seating (Bomberg et al, 1985). This often results in an uneven thickness of the impression material. Some trays are often too long or too short in relation to the extent of the oral soft and hard tissues that need to be recorded for clinical purposes and modifications to the tray need to be carried out before the trays can be used for making acceptable impressions. An initial attempt to alleviate this problem would be establishing clusters of dental arches to determine the range of impression trays that would accommodate most patients in a specific population group.

Tables 1(a) and (b), 2(a) and (b) show that the measurements obtained in this study are comparable to the measurements of other studies using the same landmarks (Hao et al., 2000; Pepe, 1975; Petričević et al., 2006). However, this study used a, b, α_2, α_1 and α_0 as indicators of shape to cluster arches and not to determine the specific shapes of dental arches, which were the objectives of other studies (Al Harbi et al., 2008; Burris and Harris, 2000; Ferrario et al., 1994).

The selection of linkage method to produce number of clusters is crucial to the objective of the study. Previous studies discussing morphology of dental arches reported about 3 to 5 different shapes based on geometrical representations (Cruz et al., 1995; Raberin et al., 1993). Therefore, the use of the complete linkage method which grouped the study sample into 2 to 6 groups was most appropriate for this study (Table 3).

To ensure that the definitive number of clusters for the population studied was deemed applicable and meaningful, three conditions had to be satisfied in order

Table 3. Number of clusters formed using the available linkage methods (M1 to M7) at selected percentage of similarity levels.

Similarity level (d_{ij}) (%)	Average(M1)	Centroid (M2)	Complete(M3)	McQuitty (M4)	Median (M5)	Single (M6)	Ward (M7)
1	1	1	2	1	1	1	9
7	1	1	2	1	1	1	10
10	1	1	2	1	1	1	10
20	1	1	3	1	1	1	11
27	1	1	3	1	1	1	11
30	1	1	4	1	1	1	12
31	1	1	4	1	1	1	12
34	1	1	4	1	1	1	12
38	1	1	5	2	1	1	12
39	1	1	5	2	1	1	12
40	1	1	5	2	1	1	12
41	1	1	5	2	1	1	12
44	1	1	6	2	1	1	14
46	1	1	6	2	1	1	14
47	1	1	6	2	1	1	15
48	1	1	6	2	1	1	15
50	1	1	6	3	1	1	16
52	2	1	6	3	1	1	16
58	3	1	9	4	1	1	19
61	4	1	10	4	2	1	20

that every cluster established had at least the minimum number of members required. In addition, the smallest margin error, *h* was necessary so that the variation between the arches in the same cluster does not differ much and therefore disparity between clusters will be more significant.

The study did not discriminate the arches according to gender, age or ethnic group. However, this information may be obtained by tracing or tracking the actual records of the subject labeled on the dendrogram. Each cluster was defined by the medians of the values used to cluster the arches and therefore may provide initial information for the design of stock impression trays for a particular population.

The study established 3 clusters (Table 4, *h*=5mm and 18 to 29% similarity level) based on the test sample. However, only 93% (37/40) of the test sample fell into the three clusters formed. The remaining 7% would be patients who would require modifications to the stock tray before use in making impressions. Due to the various designs and sizes of stock impression trays currently available commercially, knowledge of the shape and size of the arches of subjects in a certain patient population, would help dental practitioners in making informed choices regarding the selection and use of stock impression trays.

To validate that the 3 clusters are distinct, idea of analysis of variance was applied. Suppose $\underline{x}_1, \underline{x}_2, \ldots, \underline{x}_n$ represent the measurements for a given group. The first principal component of each vector, namely $\underline{x}_j$ was transformed to $\underline{v}_j = \underline{q}_j^T \underline{x}_j$, was studied. The variance (s_i^2) of the first principal component for group $i = 1,2 \text{ and } 3$ was then calculated. Finally, the sample variance s_T^2 for principal component from all groups was calculated. It is shown that $\frac{s_1^2}{s_T^2}, \frac{s_2^2}{s_T^2} \text{ and } \frac{s_3^2}{s_T^2}$ are 0.0174, 0.0405 and 0.0168 respectively, suggesting that all the clusters were distinct.

Conclusion

Within the limits of the study, it is concluded that the AHC method using $a, b, \alpha_2, \alpha_1 \text{ and } \alpha_0$ was capable of establishing 3 clusters of dental arches in the sample of Malaysian ethnic groups studied. However, the results of this study should be repeated on samples from other regions and ethnic groups before any generalizations can be made.

ACKNOWLEDGEMENT

This study was supported by Ministry of Science, Technology and Innovation (MOSTI) Malaysia Science Fund (12-02-03-2067).

Table 4. Number of clusters formed when test samples were assigned to the clusters established by the control samples.

Similarity level (%)	No of clusters	h=2mm	h=3mm	h=4mm	h=5mm	h=6mm	h=7mm
1 to 17	C1	7	13	19	26	31	37
	C2	5	6	11	7	7	3
	Total	12	19	30	33	38	40
18 to 29	C1	8	12	19	26	31	34
	C2	5	6	8	7	6	3
	C3	1	5	6	4	3	3
	Total	14	23	33	37	40	40
30 to 37	C1	7	16	21	26	32	37
	C2	0	1	1	1	1	0
	C3	5	2	7	6	3	1
	C4	1	5	5	4	4	2
	Total	13	24	34	37	40	40
38 to 42	C1	7	16	21	26	32	37
	C2	1	1	2	1	1	0
	C3	5	2	6	6	3	1
	C4	1	5	5	4	4	2
	C5	0	0	1	0	0	0
	Total	14	24	35	37	40	40
43 to 53	C1	7	16	21	26	32	37
	C2	1	1	2	1	1	0
	C3	5	3	4	7	3	1
	C4	1	5	5	4	4	2
	C5	0	0	1	0	0	0
	C6	0	2	1	0	0	0
	Total	14	27	34	38	40	40
53.50	C1	5	12	19	23	28	33
	C2	1	2	1	1	0	1
	C3	5	6	4	7	7	3
	C4	1	6	7	7	5	3
	C5	2	1	1	1	0	0
	C6	0	0	1	0	0	0
	C7	0	2	1	0	0	0
	Total	14	29	34	39	40	40
54 to 56	C1	5	12	19	23	28	33
	C2	1	2	1	1	0	1
	C3	5	6	4	7	7	3
	C4	1	6	7	7	5	3
	C5	0	1	1	1	0	0
	C6	2	1	1	1	0	0
	C7	0	0	1	0	0	0
	C8	0	2	1	0	0	0
	Total	14	30	35	40	40	40

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